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EPOXIDATION OF 1-OCTENE BY *TERT*-BUTYL HYDROPEROXIDE IN THE PRESENCE OF TITANIUM COMPOUNDS

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The epoxidation reaction of 1-octene by *tert*-butyl hydroperoxide in the presence of TiB₂, TiC and TiSi₂ was investigated. It is shown that the titanium compounds catalyzed the reaction and exhibited different activity. It is established that TiSi₂ is the best choice for the epoxidation reaction which provided 73 % of hydroperoxide conversion and 75 % of selectivity of epoxide formation. The performance of TiSi₂ after three runs indicated its excellent reusability.

Key words: epoxidation; catalyst; titanium; 1-octene; *tert*-butyl hydroperoxide.

Introduction

Epoxides have shown to be attractive, interesting and useful organic compounds [1–9]. These compounds contain highly valuable structural group namely epoxide ring. Due to that they are highly reactive and can serve as synthetic intermediates for the preparation of a large variety of compounds in organic and pharmaceutical synthesis [1–6] or as monomers in the production of various functional polymers and materials [7–9].

Epoxides can take part in a variety of nucleophilic or electrophilic reactions due to propensity of epoxide ring to open upon attack. The ring opening of epoxides has been intensively studied nowadays [1–6].

A new method for the preparation of aldols via the reaction of silyl-protected aryl cyanohydrins with epoxides has been developed [1]. β -Hydroxyketones (aldols) are prepared from the alkylation-deprotection of O-silylated aryl cyanohydrins with epoxides. Key to the success of the method was the suppression of an in situ cyclic imidate formation that occurs upon initial opening of the epoxide ring. The efficient zwitterion catalyzed epoxide ring-opening with carboxylic acids to give 1,2-diol monoesters was described in [2].

Selective hydrogenation of epoxides is a highly attractive method for preparing primary alcohols [3]. Both alkyl- and arylsubstituted epoxides were offered to apply in synthesis of primary alcohols as an alternative way of using olefins in the traditional

synthesis methods and the primary alcohols were obtained in high yields and selectivity under mild reaction conditions. So, using epoxides as substrate to synthesize primary alcohols can be considered as a promising alternative way to replace the use of alkenes.

Moreover, epoxides have found wide application in catalytic conversion of CO₂ into value-added chemicals. The cycloaddition reaction of carbon dioxide with epoxides is one of the most interesting CO₂ fixation strategies. This reaction not only has high CO₂ utilization but also produces cyclic organic carbonates and provides a low-energy catalytic pathway [4–6].

Isotacticity-rich semiaromatic polythioesters was prepared by the copolymerization of epoxides with phthalic thioanhydride [7]. Coating of wood with plant-oil based epoxide nanocomposite materials enhanced wood material densities, decreased water absorption and showed favourable qualities against mechanical effects [8]. Tensile and tear properties as well as abrasion resistance of silica natural rubber were improved after filling by epoxide [9].

Therefore, the reactions of production these useful intermediates epoxides are of growing interest. Many different methods for the preparation of epoxides are known. Among them the well-known method is the epoxidation of carbon-carbon double bond C=C by alkyl hydroperoxides using homogeneous and heterogeneous catalysts.

However, the homogeneous epoxidation method has several drawbacks such as difficulty in the separation of this catalyst from the reaction products, impossibility of their regeneration and generation of waste. The use of heterogeneous catalysts is one of the most attractive choices which could cope with most of the above mentioned drawbacks of homogeneous catalysts.

Heterogeneous transition metals compounds are outstanding catalysts in the epoxidation reaction. Among them Ti-containing compounds represent a series of promising and environmentally benign catalysts [10–20]. Atomically dispersed Ti sites on metal oxides (MO_x , including SiO_2 , $\gamma\text{-Al}_2\text{O}_3$, ZnO , GeO_2) are effective catalysts for alkene epoxidations by H_2O_2 [10].

The grafting of poly(methylhydrosiloxane) (PMHS) onto Ti/SiO_2 catalysts for improving their robustness to water, using olefin epoxidation catalysis with organic hydroperoxide as oxidant was investigated [11]. During 1-octene epoxidation reaction with *tert*-butyl hydroperoxide as oxidant under flow conditions, PMHS-16 Ti/SiO_2 exhibits almost the same activity after 50 h of time and maintains an average selectivity above 90 %. In comparison, Ti/SiO_2 and TMS Ti/SiO_2 deactivate quickly during the first ten hours of time on stream, but TMS Ti/SiO_2 shows slightly higher selectivity than PMHS-16 Ti/SiO_2 and nearly the same activity even after its deactivation, at longer times on stream. The catalytic performances of organic-inorganic hybrid $\text{C}_n\text{-Ti-HMS}$ samples prepared with various kinds of organosilanes were tested in the oil-water biphasic epoxidation of methyl oleate with H_2O_2 [12]. The methyl oleate conversion as well as selectivity to epoxidized methyl oleate over most organic-functionalized $\text{C}_n\text{-Ti-HMS}$ is higher than their inorganic counterpart Ti-HMS . Among $\text{C}_n\text{-Ti-HMS}$ methyl-functionalized $\text{C}_1\text{-Ti-HMS-50}$ displays the optimal catalytic performance with a 95 % conversion of MO, 65 % selectivity and 63 % epoxide yield. The catalytic activity of the prepared thin-walled Ti-rich hollow titanium silicalite-1 (TS-1): HTS-1#S0.25, CHTS-1 and TS-1#S0.25 zeolite were investigated on 1-hexene epoxidation reaction using H_2O_2 as an oxidant [13]. The conversion of 1-hexene is 44 % using HTS-1#S0.25 as a catalyst, with 97 % epoxide selectivity, while the conversion of 1-hexene using CHTS-1 as a catalyst is only 29 %. The HTS-1#S0.25 can be recycled by centrifugation

without any post-treatment and it remains a high oxidation activity and high selectivity after five recycle experiments.

The catalytic activities of Ti-containing periodic mesoporous organosilica (PMO) materials were tested in epoxidation of cyclohexene with an optimum conversion rate of 31 % and good epoxide selectivity of 94 % [14]. Ti-PMO materials were also effective for the epoxidation of vernonia oil by *tert*-butyl hydroperoxide with maximum percent of 48 % conversion and 94 % of epoxide selectivity. Chiral Ti-MCM-41 catalysts, prepared by grafting of $\text{Ti}(\text{O}^i\text{Pr})_4$ on MCM-41, are active in the epoxidation of styrene with *tert*-butyl hydroperoxide [15]. The solid catalysts are more active and selective than their homogeneous counterpart. Moderate enantioselectivities are obtained, with values ranging between 26 % and 71 % depending on the metal, the nature of the chiral ligand, and the calcination temperature of the support. Ti-containing hollow-structured zeolite Ti-HSZ material shows excellent catalytic activity and stability for the epoxidation of alkenes [16]. About 95 % allyl chloride can be converted into corresponding epoxide when using H_2O_2 as oxidant and about 85 % cyclopentene and 87 % cyclooctene can be converted into corresponding epoxides when using *tert*-butyl hydroperoxide as oxidant, with the selectivity for epoxides of nearly 100 %.

In [17] the epoxidation of 1,5,9-cyclododecatriene to 1,2-epoxy-5,9-cyclododecadiene with hydrogen peroxide on unmodified and on silanized Ti-SBA-15 catalyst (named as Ti-SBA-15-TMS) was described. The optimal solvent in terms of selectivity of transformation using H_2O_2 to 1,2-epoxy-5,9-cyclododecadiene was found to be 90t %. From the comparison of the activities of Ti-SBA-15 and Ti-SBA-15-TMS catalysts, it is evident that silanization decreases the rate of the epoxidation reaction but increases the selectivities of transformation of 1,5,9-cyclododecatriene and H_2O_2 to 1,2-epoxy-5,9-cyclododecadiene. Ti-BEA zeolite was investigated in detail in alkene epoxidation by H_2O_2 with or without ammonium salts [18]. It was established that when weak acidic additive (NH_4Cl) was used for alkenes epoxidation reaction catalyzed by Ti-BEA zeolite, both of the alkene conversion and 1,2-epoxide increased: from 64.0 % to 84.4 % and from 98.6 % to 99.5 % in the case of 1-hexene in acetonitrile, from 48.0 % to 63.5 % and from 98.6 % to 99.5 % in

the case of 1-hexene in acetone, from 71.8 % to 83.7 % and from 97.4 % to 99.2 % in the case of 1-octene and from 20.3 % to 88.6 % and from 92.3 % to 98.5 % in the case of 1-dodecene, respectively. The effect of different solvents with known polarity properties (CH_3CN , $(\text{CH}_3)_2\text{CO}$, CH_3OH , etc.) on the cyclohexene C_6H_{10} transformation using H_2O_2 as oxidant over Ti-Beta catalyst was described in [19]. The solvent environment affected on the reaction activity as well as product selectivity, and even the catalytic reaction mechanism. For cyclohexene C_6H_{10} the main product in CH_3CN over the Ti-Beta catalyst was determined to be epoxide $\text{C}_6\text{H}_{10}\text{O}$, while the main product in $(\text{CH}_3)_2\text{CO}$ was diol $\text{C}_6\text{H}_{12}\text{O}_2$, and the reactive activity for epoxidation is was higher in CH_3CN . BEA-Ti- H_2MTPP or BEA-Ti-MnMTPP catalysts were evaluated in the epoxidation of cyclohexene by *tert*-butyl hydroperoxide [20]. Differences in the selectivity were detected when BEA-Ti- H_2MTPP or BEA-Ti-MnMTPP was applied in the epoxidation of cyclohexene. The combination of BEA-Ti- H_2MTPP and porphyrin afforded cyclohexene oxide with high selectivity (cyclohexene oxide / 2-cyclohexen-1-one=85:15), while the integration of BEA-Ti-MnMTPP yielded 2-cyclohexen-1-one with high selectivity (cyclohexene oxide / 2-cyclohexen-1-one=12:88).

The aim of the work is to investigate the epoxidation reaction of 1-octene by *tert*-butyl hydroperoxide in the presence of titanium compounds as heterogeneous catalysts to determine their catalytic activity.

Materials and research methods

1-octene (OK) and 1,2-epoxyoctane (EPO) obtained from Aldrich. Chlorbenzene, reagent chemically pure grade. 1-Octene and chlorbenzene were additionally dried and distilled. *Tert*-butyl hydroperoxide (TBHP) was synthesized by [21]. TiB_2 , TiC and TiSi_2 were commercial chemicals of chemically pure grade of Donetsk factory of chemical reagents with BET surface area $1.1 \text{ m}^2/\text{g}$, $1.2 \text{ m}^2/\text{g}$ and $1.3 \text{ m}^2/\text{g}$, respectively.

Octene-1, TBHP, chlorbenzene and catalyst were added to the thermostated glass reactor and the epoxidation reaction was carried out at 388 K under argon argon atmosphere and stirring with rate of 1000 rpm in kinetic regime of the process. Initial concentrations OK and TBHP were 4 mol/l and 0.5 mol/l, catalyst content was $4 \text{ m}^2/\text{l}$. In definite intervals the samples of reaction mixture were withdrawn

to analyze. TBHP concentration was determined by iodometric titration. The reaction mixture was analyzed by chromatographic method. Additionally it was established uncatalytic decomposition of hydroperoxide as well as epoxide formation practically did not proceeded.

Percent of conversion of *tert*-butyl hydroperoxide, selectivity of 1,2-epoxycyclooctane formation and yield of 1,2-epoxycyclooctane were calculated in the following way:

$$\text{Conversion, \%} = 100 \cdot [\text{TBHP reacted}] / [\text{TBHP initial}].$$

$$\text{Selectivity, \%} = 100 [\text{EPO formed}] / [\text{TBHP reacted}].$$

$$\text{Yield, \%} = 100 [\text{EPO formed}] / [\text{TBHP initial}].$$

Results and discussion

Figs. 1 and 2 show the proceeding of the epoxidation reaction of 1-octene by *tert*-butyl hydroperoxide in the presence of titanium compounds namely TiB_2 , TiC and TiSi_2 .

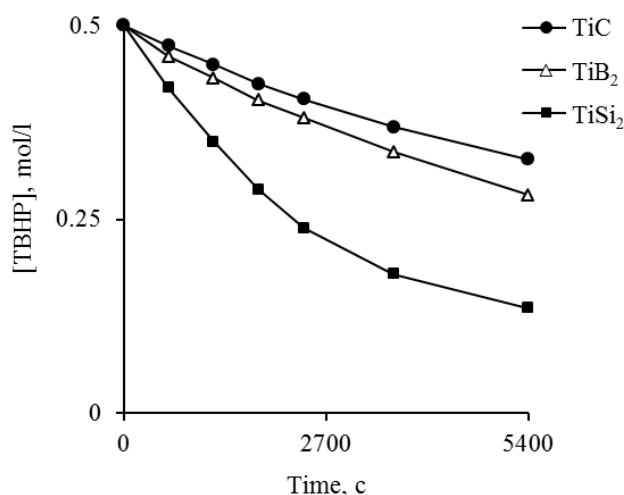


Fig. 1. Kinetic curves for *tert*-butyl hydroperoxide consumption in the 1-octene epoxidation reaction in the presence of titanium compounds namely TiB_2 , TiC and TiSi_2

It is seen that the most active TBHP consumed and 1,2-epoxyoctane accumulated in the presence of titanium silicide. The kinetic curves of TBHP consumption as well as kinetic curves of epoxide accumulation in the presence of titanium carbide and boride are close and these processes proceed worse in compare with the same in the presence of titanium silicide. Moreover, the lowest hydroperoxide consumption is observed for TiC, while the lowest amount of formed epoxide for TiB_2 .

Catalytic performance of titanium compounds are presented in Fig. 3–5.

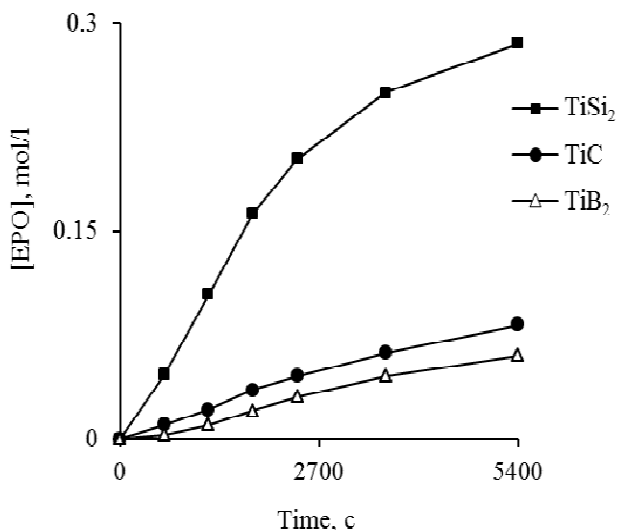


Fig. 2. Kinetic curves for 1,2-epoxyoctane accumulation in the epoxidation reaction of 1-octene by tert-butyl hydroperoxide in the presence of TiB_2 , TiC and $TiSi_2$

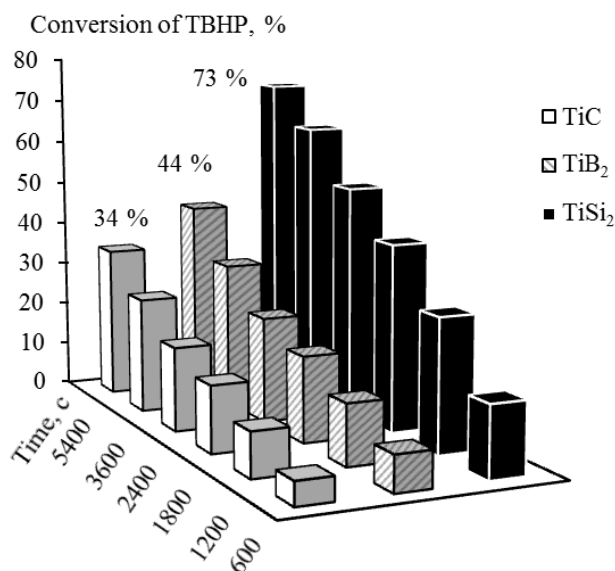


Fig. 3. Evolution of conversion of tert-butyl hydroperoxide in the epoxidation reaction of 1-octene using titanium compounds

From Fig. 3 one can see that TBHP conversion reach the value of 73 % in 90 min of reaction proceeding and is the highest for $TiSi_2$, whereas for TiB_2 it is equal to 44 % and for TiC – 34 %.

Selectivity of epoxide formation (Fig. 4) for $TiSi_2$ and TiC is 77 % and 47 % respectively and this value is reach already in 30 min and remain the same for next investigated time diapason. In the case of TiB_2 the selectivity of 27 % is reach only in 40 min of reaction and as in the case of $TiSi_2$ and TiC does not vary.

The highest yield of 1,2-epoxyoctane in the reaction of hydroperoxide epoxidation of 1-octene (Fig. 5) is obtained for titanium silicide and equaled to 57 %, for titanium carbide and boride it's value is close and equal to 16 and 12 % respondingly.

In the presence of titanium compounds the values of the epoxidation reaction parameters varies as:

TBHP conversion: $TiC < TiB_2 < TiSi_2$;

selectivity for 1,2-epoxyoctane formation:

$TiB_2 < TiC < TiSi_2$;

1,2-epoxycyclooctane yield: $TiB_2 \leq TiC < TiSi_2$.

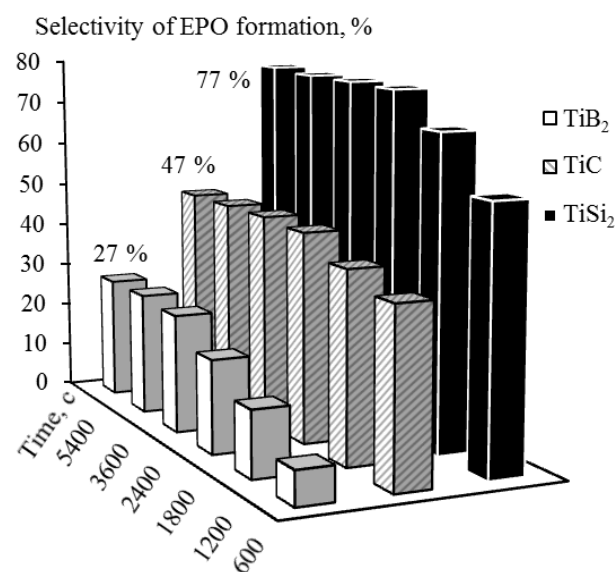


Fig. 4. Evolution of selectivity of 1,2-epoxycyclooctane formation in the hydroperoxide epoxidation reaction of 1-octene using titanium compounds

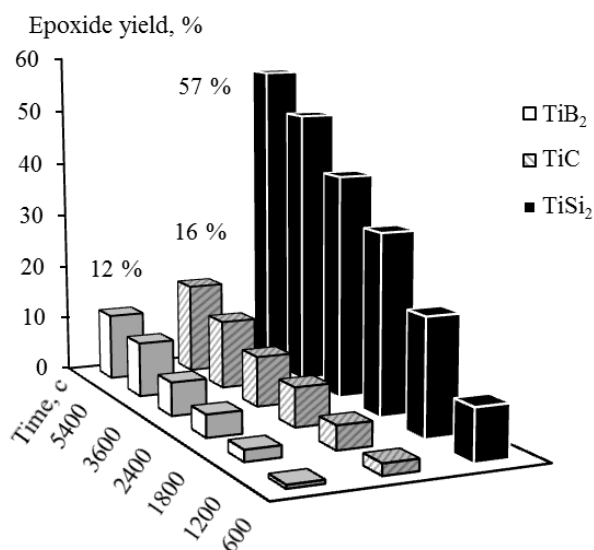


Fig. 5. Evolution of yield of 1,2-epoxycyclooctane in the hydroperoxide epoxidation reaction of 1-octene using titanium compounds

The obtained experimental results show that all investigated titanium compounds catalyze the epoxidation process of 1-octene by *tert*-butyl hydroperoxide. However, part of TBHP remain either unreacted or unincorporated in epoxide ring formation and decompose.

In order to get insight into that process the bar charts of hydroperoxide consumption are presented in Figs. 6–8.

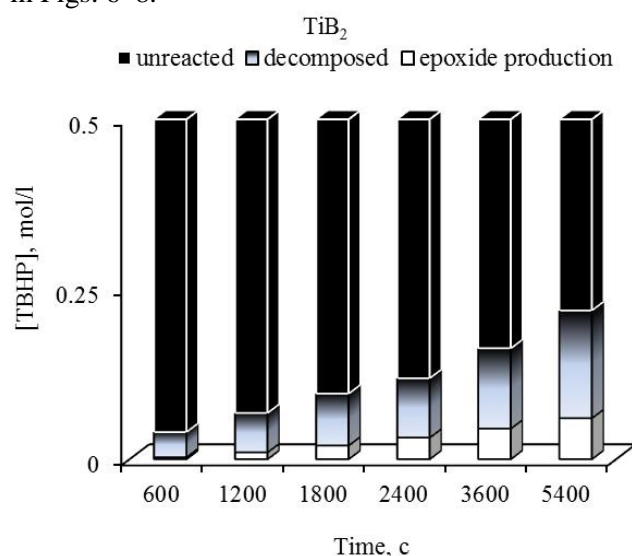


Fig. 6. Evolution of the part of tert-butyl hydroperoxide consumed for 1,2-epoxycyclooctane production and as well as decomposed without formation of epoxide and unreacted hydroperoxide in the epoxidation reaction of 1-octene in the presence of TiB₂

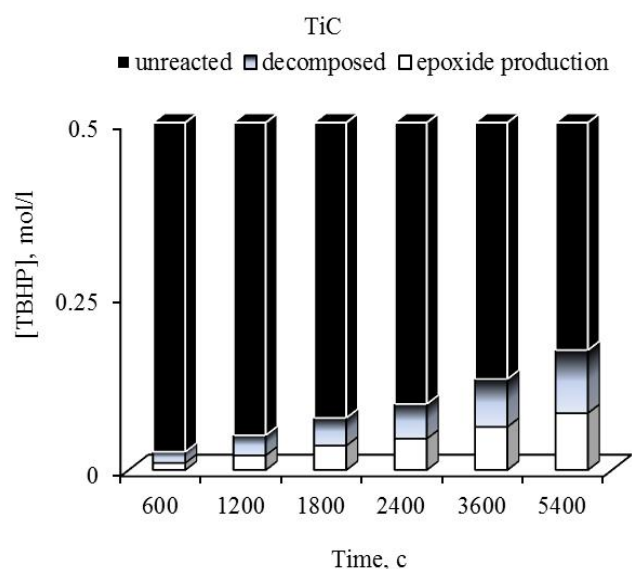


Fig. 7. Evolution of the part of tert-butyl hydroperoxide consumed for 1,2-epoxycyclooctane production and as well as decomposed without formation of epoxide and unreacted hydroperoxide in the epoxidation reaction of 1-octene in the presence of TiC

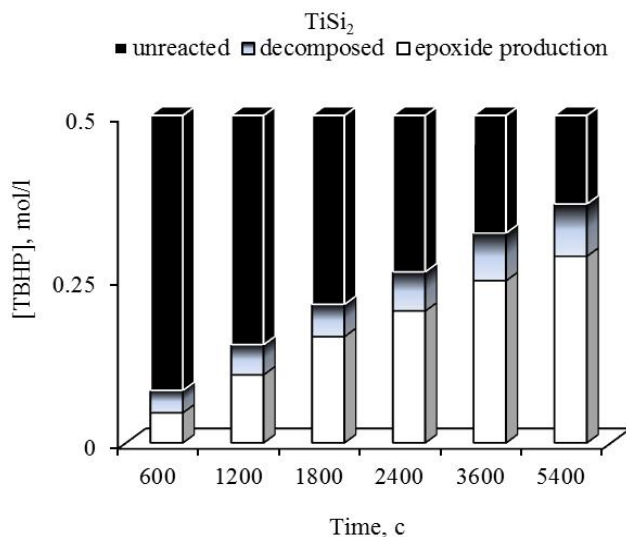


Fig. 8. Evolution of the part of tert-butyl hydroperoxide consumed for 1,2-epoxycyclooctane production and as well as decomposed without formation of epoxide and unreacted hydroperoxide in the epoxidation reaction of 1-octene in the presence of TiSi₂

The smallest amount of as unreacted TBHP as decomposed hydroperoxide without epoxide production is observed in the presence of titanium silicide (Fig. 8). In the case of titanium boride the smallest amount of TBHP composed for epoxide formation, in 4.7 times lower than in the case of titanium silicide, and the largest TBHP amount composed for decomposition, twice higher than the same for titanium silicide. The largest amount of unreacted hydroperoxide is in the case of titanium carbide, in 2.4 times higher than for titanium silicide.

According to TBHP path consumed the investigated titanium catalysts can be put in the order:

unreacted TBHP: $\text{TiSi}_2 < \text{TiB}_2 < \text{TiC}$;

decomposed HPTB: $\text{TiSi}_2 < \text{TiC} < \text{TiB}_2$;

HPTB for epoxide production: $\text{TiB}_2 < \text{TiC} < \text{TiSi}_2$.

Among investigated titanium compounds TiSi_2 is a preferable catalyst for the hydroperoxide epoxidation reaction of 1-octene.

Therefore, the recyclability of this most active Ti-catalyst, TiSi_2 , was evaluated in the recycling test consisting of three runs and the results are shown in Figs. 9, 10. After each cycle the sample of TiSi_2 was collected, dried, and then used in the next cycle. It was found that after the second cycle the TBHP conversion as well as selectivity of epoxide formation remained the same. Only after the third cycle the slightly decrease in TBHP conversion from 73 % to 71 % and selectivity from 77 % to 75 % was observed. The obtained results verified the sustainable catalytic activity of TiSi_2 in the epoxidation of 1-octene by *tert*-butyl hydroperoxide.

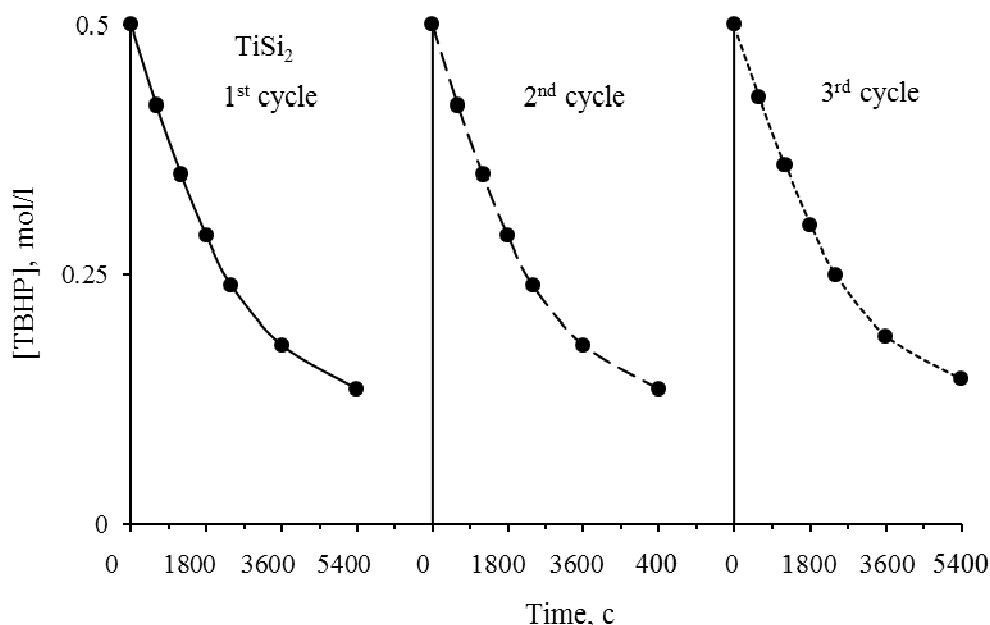


Fig. 9. The reusability of TiSi_2 catalyst for the epoxidation reaction of 1-octene by TBHP for three cycles

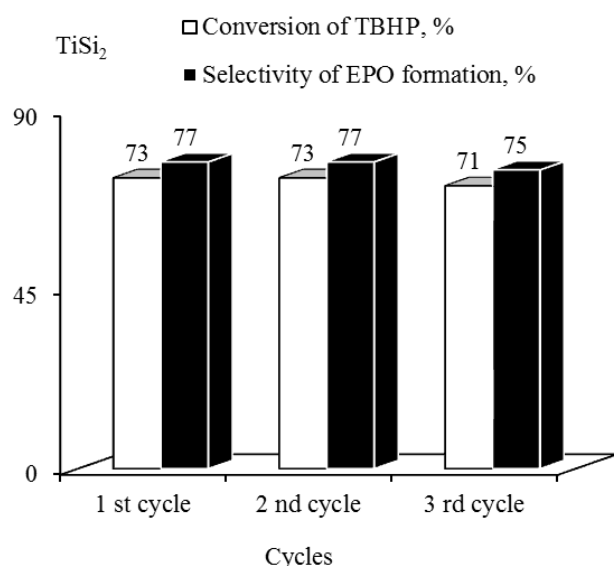


Fig. 10. Results of recycling tests of catalytic performance of TiSi_2 for the hydroperoxide epoxidation reaction of 1-octene

Thus, Ti-compounds demonstrate different catalytic activity of in the epoxidation reaction of 1-octene. Among them TiSi_2 is the best catalysts for epoxidation reaction.

Conclusions

The epoxidation reaction of 1-octene by *tert*-butyl hydroperoxide in the presence of titanium compounds was investigated. TiSi_2 is the most active, whereas both TiB_2 and TiC exhibit lower catalytic activity. The selectivity of epoxide formation in the presence of TiSi_2 ,

TiC and TiB_2 reach values 77 %, 47 % and 37 %, respectively. TiSi_2 shows an excellent reusability with the selectivity of epoxide formation of 75 % after three runs.

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ЕПОКСИДУВАННЯ ОКТЕНУ-1 ТРЕТ-БУТИЛГІДРОПЕРОКСИДОМ У ПРИСУТНОСТІ СПЛУК ТИТАНУ

Досліджено реакцію епоксидування октену-1 гідропероксидом *трет*-бутилу в присутності TiB₂, TiC і TiSi₂. Показано, що сполуки титану каталізують реакцію і проявляють різну активність. Встановлено, що TiSi₂ є найкращим каталізатором для реакції епоксидування: забезпечує конверсію гідропероксиду 73 % і селективність утворення епоксиду 75 %. Показано можливість повторного використання TiSi₂ протягом трьох циклів.

Ключові слова: епоксидування; каталізатори; титан; октен-1; гідропероксид *трет*-бутилу.